

Using Structural Docking for Drug Repurposing

Abstract:

Recently the FDA has increased restrictions making it very difficult to get a new drug out. Therefore it is desirable to repurpose a drug already in use, one which has passed clinical studies and has few side effects. For this reason we created a method to repurpose existing drugs to treat diseases other than their known targets. In this study we chose to demonstrate our method on colorectal cancer. CRC is an interesting disease for this approach, as known CRC chemotherapy drugs are ineffective in curing this kind of cancer. To find repurposed drugs for CRC we first use a structural algorithm to identify probable CRC gene targets for a specific set of in market cancer drugs. After prioritizing these targets, the relationships between the gene targets and the potential drugs are validated and scored using Autodock. We can then identify which drugs have the greatest potential of being repurposed to treat CRC. It is our hope that this method will be able to aid in finding new treatments for diseases without the cost and risk of developing new drugs.